

Classical diffusion of N interacting particles

in one dimension: General results and asymptotic laws

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I consider the coupled one-dimensional diffusion of a cluster of N classical particles with contact repulsion. General expressions are given for the probability distributions, allowing to obtain the transport coefficients. In the limit of large N , and within a gaussian approximation, the diffusion constant is found to behave as N^{-1} for the central particle and as $(\ln N)^{-1}$ for the edge ones. Absolute correlations between the edge particles *increase* as $(\ln N)^2$. The asymptotic one-body distribution is obtained and discussed in relation of the statistics of extreme events.

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I. INTRODUCTION

Low dimensionality, geometrical constraints and interactions between classically diffusing particles are expected to modify transport coefficients and/or the nature of the asymptotic regimes. As a trivial example, a brownian particle subjected to a purely reflecting wall has a anomalous drift, its average position increasing as $t^{1/2}$, (which corresponds to a vanishing velocity) whereas the centered second moment has a normal diffusive spreading with a lowered diffusion constant as compared to the diffusion without barrier. In the case of two particles with a contact repulsion, each of them plays for the other the role of a *fluctuating* boundary condition which affects both the transport coefficients linked to the average position and the mean square deviation. The aim of this letter is to discuss such questions in the general case of N mutually interacting particles with a hard-core interaction.

Classical diffusion with interactions does not seem to have drawn so much attention. A notable exception is the so-called “tracer problem” defined as the diffusion of a tagged particle in an infinite sea of other diffusing particles. The one-dimensional model was first solved by Harris¹ and discussed in subsequent papers^{2,3}. The main result is that the mean square dispersion of the position, Δx^2 , displays a subdiffusive behaviour, which originates from the fact

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that the motion of the tagged particle is, anywhere and at any time, hindered by all surrounding particles. In one dimension Harris found that Δx^2 grows as $t^{1/2}$ at large times; this implies that the typical distance travelled by the tracer at time t goes like $t^{1/4}$ instead of $t^{1/2}$ in the free case. More recently, Derrida et al.⁴ found several exact results for the asymmetric simple exclusion process⁵; recent bibliography and other results on such subject can be found in Mallick's thesis⁶.

The problem here considered is frankly different, although it belongs to the so-called single-file diffusion problem encountered in many fields (one-dimensional hopping conductivity⁷, ion transport in biological membranes^{8,9}, channelling in zeolites¹⁰). At some initial time, a compact cluster of N pointlike particles is launched at the origin of a one-dimensional space; each of them undergoes ordinary brownian motion but has a contact repulsive interaction with its neighbours. As a consequence, the particles located at the edge of the cluster can move freely on one side and are subjected to a fluctuating boundary condition on the other, whereas the particles inside the cluster are subjected to such boundary conditions on either side.

The questions to be solved are to find the (anomalous) drift of one particle and its diffusion constant as a function of the position within the cluster and of the number of N . In addition, two-particle correlations are worthy to be analyzed, as well as the asymptotic one-body probability distributions.

II. ONE-PARTICLE TRANSPORT COEFFICIENTS

At the initial time, the N particles are assumed to form a compact cluster located at the origin $x = 0$, each of them having the same diffusion constant D as all the others. Due to the contact repulsion, two particles can never cross each other, so that order in space is preserved at any time; this means that the N coordinates x_i can be labelled so that:

$$x_1 < x_2 < \dots < x_N \quad \forall t . \quad (2.1)$$

The solution of the diffusion equation for such an initial condition is the following:

$$p(x_1, x_2, \dots, x_N; t) = N! \prod_{n=1}^N \frac{e^{-x_n^2/(4Dt)}}{\sqrt{4\pi Dt}} \prod_{n=1}^{N-1} Y(x_{n+1} - x_n) , \quad (2.2)$$

where Y is the Heaviside unit step function ($Y(x) = 1$ if $x > 0$, 0 otherwise). In a recent and important paper¹¹, the general formal solution of the same problem with an arbitrary initial condition was given, using the reflection principle. From eq. (2.2), one readily gets the reduced one-particle density for the n^{th} particle of the cluster:

$$p_n^{(1)}(x; t) = \frac{2^{1-N} N!}{(n-1)!(N-n)!} \left[1 + \Phi \left(\frac{x}{\sqrt{4Dt}} \right) \right]^{n-1} \left[1 - \Phi \left(\frac{x}{\sqrt{4Dt}} \right) \right]^{N-n} \frac{e^{-x^2/(4Dt)}}{\sqrt{4\pi Dt}} . \quad (2.3)$$

In the last equation, Φ denotes the probability integral¹², satisfying $\Phi(\pm\infty) = \pm 1$. The two factors $(1 \pm \Phi)$ represent the steric effects on the n^{th} particle due to the other ones. Knowing $p_n^{(1)}$, it is in principle possible to compute the first few moments giving the average position and the mean square dispersion for anyone of the particles. As a first result, one immediately observes that any moment of the coordinate has a quite simple variation in time, at any time, not only in the final stage of the motion. Indeed, using eq. (2.3), it is readily seen that the k^{th} moment $\langle x_n^k \rangle$ increases at any time as $t^{k/2}$ since $(Dt)^{1/2}$ is the only lengthscale of the problem. As a consequence, $\forall t$, the average coordinate of the n^{th} particle $\langle x_n \rangle(t)$ increases as $t^{1/2}$ – except for instance for the central particle of the cluster when N is odd –, whereas the mean square displacement $\Delta x_n^2 \equiv \langle x_n^2 \rangle - \langle x_n \rangle^2$ increases as t . The drift, due to left-right symmetry breaking, is thus always anomalous and the diffusion is always normal. As a consequence, one can define, $\forall n$ and N , the following transport coefficients $V_{1/2, n}$ and D_n :

$$\langle x_n \rangle = V_{1/2, n}(N) t^{\frac{1}{2}} , \quad (2.4)$$

$$\Delta x_n^2 = 2D_n(N) t , \quad (2.5)$$

It remains to find the functions $V_{1/2, n}(N)$ and $D_n(N)$, which incorporate the dependence of the transport coefficients upon the number of particles. For $N = 2$, one readily finds:

$$\langle x_2 \rangle = - \langle x_1 \rangle = \sqrt{\frac{2}{\pi}} Dt , \quad (2.6)$$

and

$$\Delta x_n^2 = 2\left(1 - \frac{1}{\pi}\right) t . \quad (2.7)$$

In the case of a non-fluctuating (fixed) perfectly reflecting barrier, one has:

$$\langle x \rangle = \sqrt{\frac{4}{\pi}} Dt \quad \Delta x^2 = 2\left(1 - \frac{2}{\pi}\right) t . \quad (2.8)$$

Thus, for a cluster of two particles, each of them acting for the other as a fluctuating barrier, the drift is slowed and the diffusion is enhanced as compared to a fixed barrier. These facts are easily understood on physical grounds.

Unfortunately, it does not seem possible to write the exact expressions of $V_{1/2, n}$ and D_n in a closed, tractable form, starting from eq. (2.3). On the other hand, since it is worthy to analyze the case of a large number $N \gg 1$ and

since the factors involving the Φ 's functions have rather sharp derivatives, especially when N is large, it is expected that a gaussian approximation can indeed produce the correct large- N variation of the $V_{1/2, n}$ and D_n .

Let us first consider one of the two particles located at one extremity of the cluster, the right one for instance. From eq. (2.3), the one-body density can be written as ($u = x/\sqrt{4Dt}$):

$$p_N^{(1)}(x; t) = \frac{1}{\sqrt{4Dt}} \frac{d}{du} \left[\frac{1 + \Phi(u)}{2} \right]^N . \quad (2.9)$$

This expression naturally has the form encountered in the statistics of extreme values¹³. When $N \gg 1$, this is a very sharp function with a maximum u_0 defined by:

$$\frac{e^{-u_0^2}}{u_0} \simeq \frac{2\sqrt{\pi}}{N} . \quad (2.10)$$

Making now a gaussian approximation for $p_N^{(1)}(x; t)$, one readily finds, up to logarithmic corrections:

$$\langle x_N \rangle = - \langle x_1 \rangle \simeq \sqrt{\ln \frac{N}{2\sqrt{\pi}}} \sqrt{4Dt} . \quad (2.11)$$

Thus, for large N , the coefficient for the anomalous drift has a logarithmic increase with respect to the number N of particles of the cluster:

$$V_{1/2 N}(N) \propto (\ln N)^{1/2} . \quad (2.12)$$

The fact that $V_{1/2 N}$ increases with N is evident on physical grounds (all the “inside” particles are pushing on those which are at the edges), but this increase is extremely slow. In addition, the same approximation yields:

$$\Delta x_N^2 = \Delta x_1^2 \simeq \frac{e^{2/3}}{(2\pi)^{1/3} \ln \frac{N}{2\sqrt{\pi}}} Dt , \quad (2.13)$$

so that:

$$D_1(N) = D_N(N) \propto (\ln N)^{-1} . \quad (2.14)$$

Although the diffusion is normal, the diffusion constant decreases and tends toward 0 for infinite N . In a pictorial way, the more there are particles pushing on its back, the less quickly spreads any one of the edge particles on either side of its average position, which drifts proportionally to $t^{1/2}$. Note that, from eqs. (2.11) and (2.13), the relative fluctuations for the edge particles behave as $(\ln N)^{-1}$; this extremely slow decrease of fluctuations, as compared to $N^{-1/2}$ in ordinary cases, implies that convergence toward a large-number law, if any, is quite poor.

The correctness of the gaussian approximation for the two first moments was checked by numerically computing the exact average position and exact mean square displacement and by looking at $\langle x_N \rangle / [4Dt \ln(N/2\sqrt{\pi})]^{1/2}$ and

$[\Delta x_N^2/(4Dt)] \ln \frac{N}{2\sqrt{\pi}}$. Fig. 1 displays the rather rapid convergence of such quantities toward constants at large N , confirming the validity of the gaussian approximation at least for the two first moments.

Obviously, things go quite differently for the particle located at the center of the cluster, assuming N to be an odd number for simplicity. First, it does not move in the mean. Second, it must have a rather small diffusion constant as compared to the edge particles, since it is strongly inhibited by its numerous erratic partners on either side of it. Indeed, the gaussian approximation yields:

$$\Delta x_{(N+1)/2}^2 \simeq \frac{\pi}{N} Dt . \quad (2.15)$$

This provides the large- N dependence of the diffusion constant for the central particle:

$$D_{(N+1)/2}(N) \propto \frac{1}{N} , \quad (2.16)$$

entailing that the fluctuations are now of the order of $1/\sqrt{N}$.

Thus, in any case, the diffusion is normal, as contrasted to the Harris' case for which $\Delta x^2 \propto t^{1/2}$. Yet, note that in the $N \rightarrow \infty$ limit, both D_N and $D_{(N+1)/2}$ vanish, which indicates a lowering of the dynamical exponent. The vanishing in all cases of the diffusion constants in the N -infinite limit signals the onset of a subdiffusive regime in the finite concentration situation. Considering the middle particle, which is surrounded by infinitely many other, this is in conformity with Harris' result. For the two edge particles, the marginal logarithmic decrease of D_N comes from the fact that the former still face a free semi-infinite space to wander in.

Note that the scaling upon N as described by eqs. (2.12) and (2.14) are the same as those obtained in ref.¹⁴; nevertheless, the asymptotic distribution law is not of the Gumbel type (see below).

III. CORRELATIONS

Statistical correlations inside the cluster are also worthy to analyze. As an example, let us consider the correlations between the two edge particles. For the latter, the two-body probability density is easily found from eq. (2.2) as the following:

$$p_{1N}^{(2)}(x_1, x_N; t) = \frac{N(N-1)}{\pi 2^N Dt} [\Phi(u_N) - \Phi(u_1)]^{N-2} e^{-(u_1^2 + u_N^2)} Y(u_N - u_1) . \quad (3.17)$$

Two-body correlations are most simply measured by $C_{1N} = \langle x_1 x_N \rangle - \langle x_1 \rangle \langle x_N \rangle$; making again a gaussian approximation for the two-body density, this correlator has the following approximate expression:

$$C_{1N}(t) \simeq 4 \ln \frac{N}{2\sqrt{\pi}} Dt . \quad (3.18)$$

Due to scaling in space, the normalized ratio $C_{1N}(t)/\Delta x_1^2$ is a constant in time. This constant turns out to be an *increasing* function of the number N of particles; from eqs. (2.11) and (2.13), one finds:

$$\frac{C_{1N}(t)}{\Delta x_1^2} \simeq 4 \left(\frac{2\pi}{e^2} \right)^{1/3} \left[\ln \frac{N}{2\sqrt{\pi}} \right]^2 . \quad (3.19)$$

Thus, increasing the number of inner particles *enhances*, although quite slowly, the correlations between the two edge particles. Far from inducing some kind of screening effect, repeated numerous collisions from inner particles enhance the statistical correlations between the edge particles. In a pictorial way, it can be said that the former act as “virtual bosons” by going from one to the other edge particles; the more they are, stronger is the effective (statistical) coupling.

IV. ASYMPTOTIC DISTRIBUTION LAWS

Interestingly enough, it is also possible to obtain the asymptotic form of the one-body distribution given by eq. (2.3). For the right particle ($n = N$), starting from eq. (2.9), one easily finds, with still $u = x/\sqrt{4Dt} > 0$:

$$p_N^{(1)}(x, t) \simeq \frac{N}{\sqrt{4\pi Dt}} \left(1 + \frac{1}{2u^2} \right) \exp \left[-u^2 - \frac{N}{2u\sqrt{\pi}} e^{-u^2} \right] . \quad (4.20)$$

The maximum occurs for $u \simeq u_0$ and the front is clearly asymmetric around u_0 – although the gaussian approximation, as shown above, well accounts for the large- N dependence of the two first moments (expectation value and fluctuations). This asymmetry represents the pressure exerted by the inner particles on the edge ones. For the left particle, one simply has $p_1^{(1)}(x, t) = p_N^{(1)}(-x, t)$. Fig. 2 shows that the large- N expression, eq. (4.20), reproduces quite well the exact $p_N^{(1)}$ even for a moderately large value of N . From eq. (4.20), it is seen that $p_N^{(1)}(x, t)$ is not exactly a Gumbel distribution; on the other hand, the rescaled variable $u^2 - \ln(N/2\sqrt{\pi})$ has, up to logarithmic corrections, the same dependence upon N as a true Gumbel variable as far as the two first moments are concerned.

As contrasted, starting again from eq. (2.3) for the central particle ($n = (N + 1)/2$), the asymptotic form of the one-body density turns out to be simply the following normal law:

$$p_{(N+1)/2}^{(1)}(x, t) \simeq \frac{1}{\pi} \sqrt{\frac{N}{2Dt}} e^{-Nx^2/(2\pi Dt)} , \quad (4.21)$$

in agreement with eq.(2.15).

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Figure Captions

1. Illustration of the asymptotic dependence upon N of the transport coefficients for the edge particles (average position, eq. (2.11) and mean square displacement, eq. (2.13)).
2. Comparison of the exact (solid line) and asymptotic distribution (dashed line) functions, respectively given by eqs. (2.3) and (4.20), for a cluster of 1000 particles; the abscissa is the reduced variable $u = x/\sqrt{4Dt}$.



